

Dichloroacetylene
7572-29-4 | DTXSID7020429

Model Performance

Model

Data

Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.79

Global applicability domain: Outside

Local applicability domain index: 3.24e-01

Confidence level: 6.02e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2,3-Dibromothiophene</div> <div>Measured: 3.53</div> <div>Predicted: 3.53</div>	<div>Image not found</div> <div>Tetrachloroethylene</div> <div>Measured: 3.40</div> <div>Predicted: 3.35</div>	<div>Image not found</div> <div>3-Bromothiophene</div> <div>Measured: 2.62</div> <div>Predicted: 2.10</div>
<div>Image not found</div> <div>Trichloroethylene</div> <div>Measured: 2.42</div> <div>Predicted: 2.29</div>	<div>Image not found</div> <div>1,2-Dibromoethylene</div> <div>Measured: 1.76</div> <div>Predicted: 1.90</div>	